INTERNATIONAL CAE CONFERENCE

LET'S SIMULATE
THE WORLD
OF THE FUTURE

21 – 22 October 2013
Pacengo del Garda, Verona - ITALY

Towards smart hydrogen economy: solar-to-hydrogen open and hybrid cycles

Michael Gasik
Aalto University Foundation, Finland

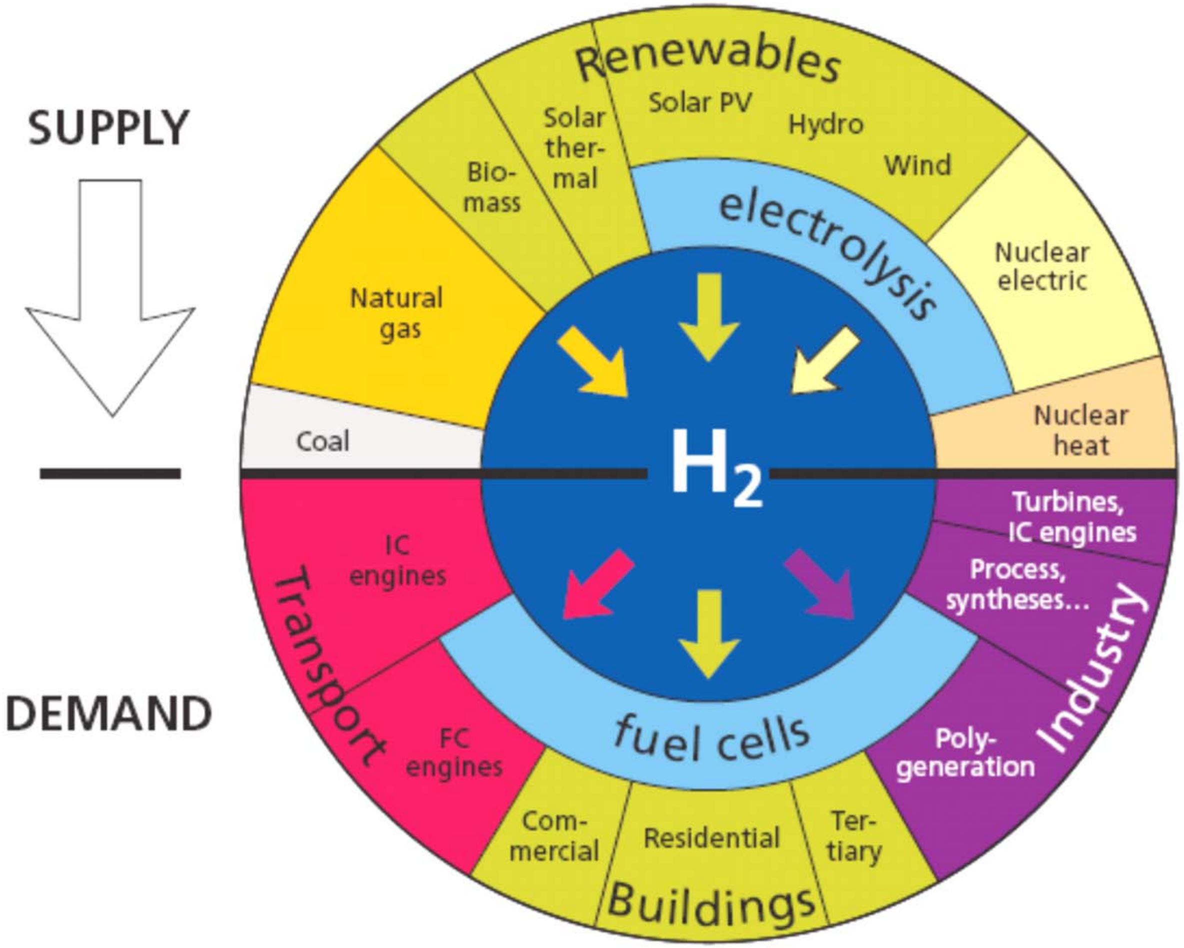
European energy policy

By 2020, replace 20% of petroleum fuels with:

<2% hydrogen

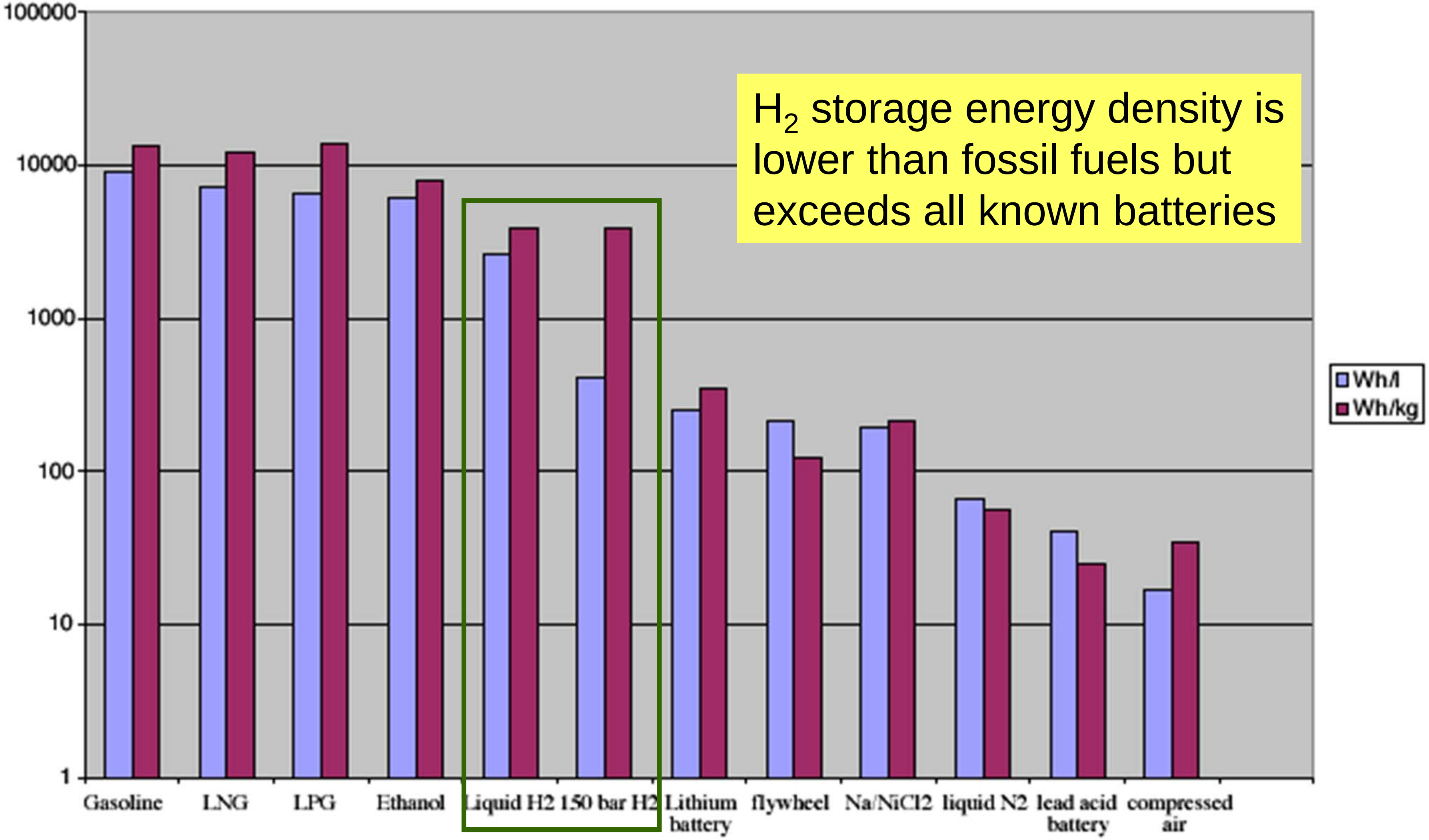
5-8% biofuels

10% natural gas



Source: European natural gas vehicle association; FCH JU; European Commission

Energy density – storage comparison



H_2 storage energy density is lower than fossil fuels but exceeds all known batteries

How to make hydrogen?

Hydrogen production technology	Benefits	Barriers
Electrolysis: splitting water using electricity	Commercially available with proven technology; Well-understood industrial process; modular; high purity hydrogen, convenient for producing H_2 from renewable electricity, compensates for intermittent nature of some renewables	Competition with direct use of renewable electricity
Reforming (stationary and vehicle applications): splitting hydrocarbon fuel with heat and steam	Well-understood at large scale; widespread; low-cost hydrogen from natural gas; opportunity to combine with large scale CO_2 sequestration ('carbon storage')	Small-scale units not commercial; hydrogen contains some impurities - gas cleaning may be required for some applications; CO_2 emissions; CO_2 sequestration adds costs; primary fuel may be used directly
Gasification: splitting heavy hydrocarbons and biomass into hydrogen and gases for reforming	Well-understood for heavy hydro-carbons at large scale; can be used for solid and liquid fuels; possible synergies with synthetic fuels from bio-mass- biomass gasification being demonstrated	Small units very rare; hydrogen usually requires extensive cleaning before use; biomass gasifica-tion still under research; biomass has land-use implications; competition with synthetic fuels from biomass
Thermochemical cycles using cheap high temperature heat from nuclear or concentrated solar energy	Potentially large scale production at low cost and without greenhouse gas emission for heavy industry or transportation; International collaboration (USA, Europe and Japan) on research, development and deployment	Complex, not yet commercial, research and development needed over 10 years on the process: materials, chemistry technology; High Temperature nuclear reactor (HTR) deploy-ment needed, or solar thermal concentrators
Biological production: algae and bacteria produce hydrogen directly in some conditions	Potentially large resource	Slow hydrogen production rates; large area needed; most appropriate organisms not yet found; still under research

Cycles comparison: visualisation

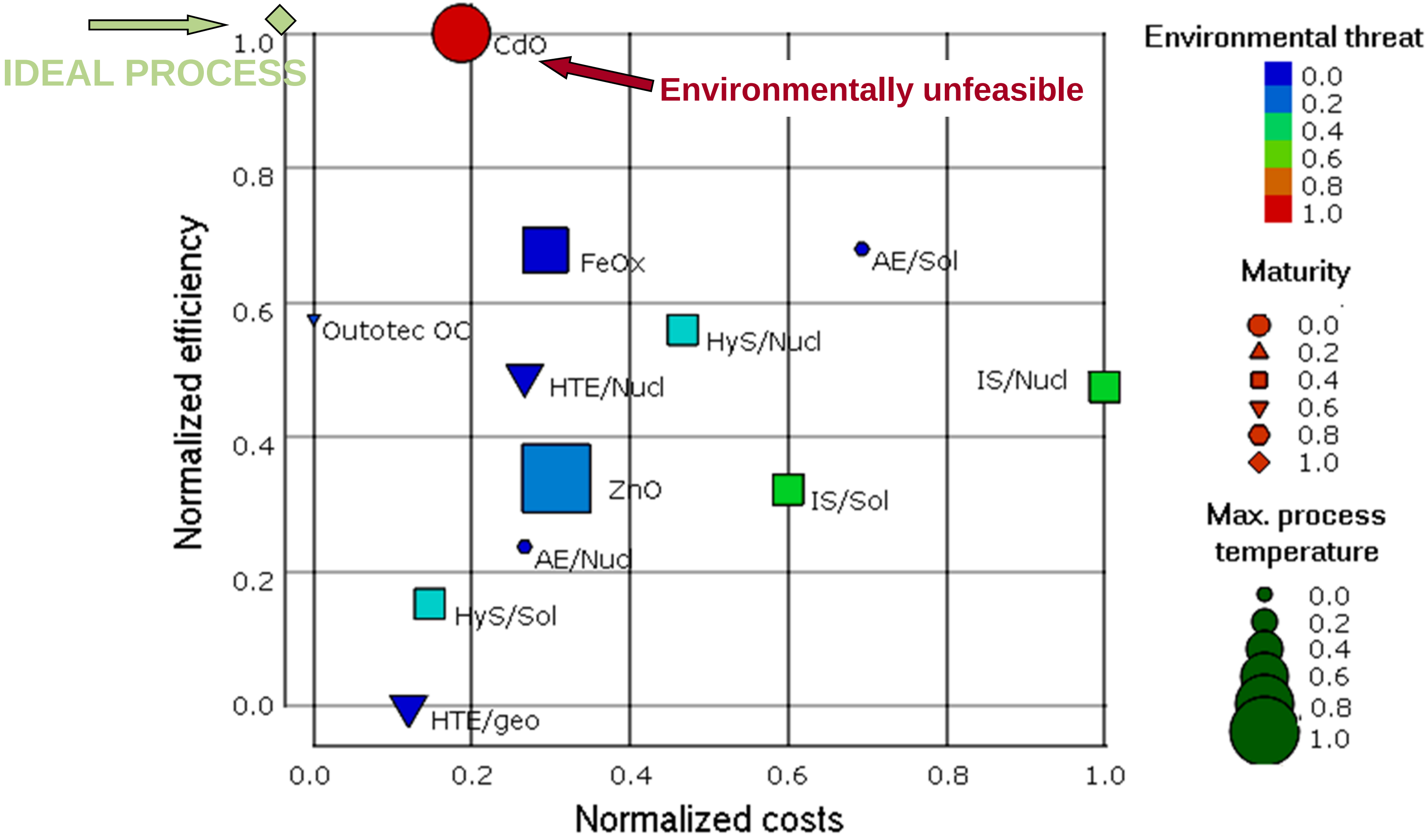
- Goal: to extract **useful information** for human eyes
- Mapping the dataset onto a 3-D space preserving distance information of the original dataset as much as possible.
- Making partitioning of complex datasets into less complex pieces and presenting them in a non-overlapping manner so regularities or irregularities could be seen
- In this case using **Grapheur** software (*by Reactive Search*)

✓ able to **discover hidden correlations** between parameters and to evaluate experimental data critically in respect to **outliers and possible errors.**

✓ **does not postulate any model** for the interaction parameters neither require any fitting parameters to provide interpolation and extrapolation.

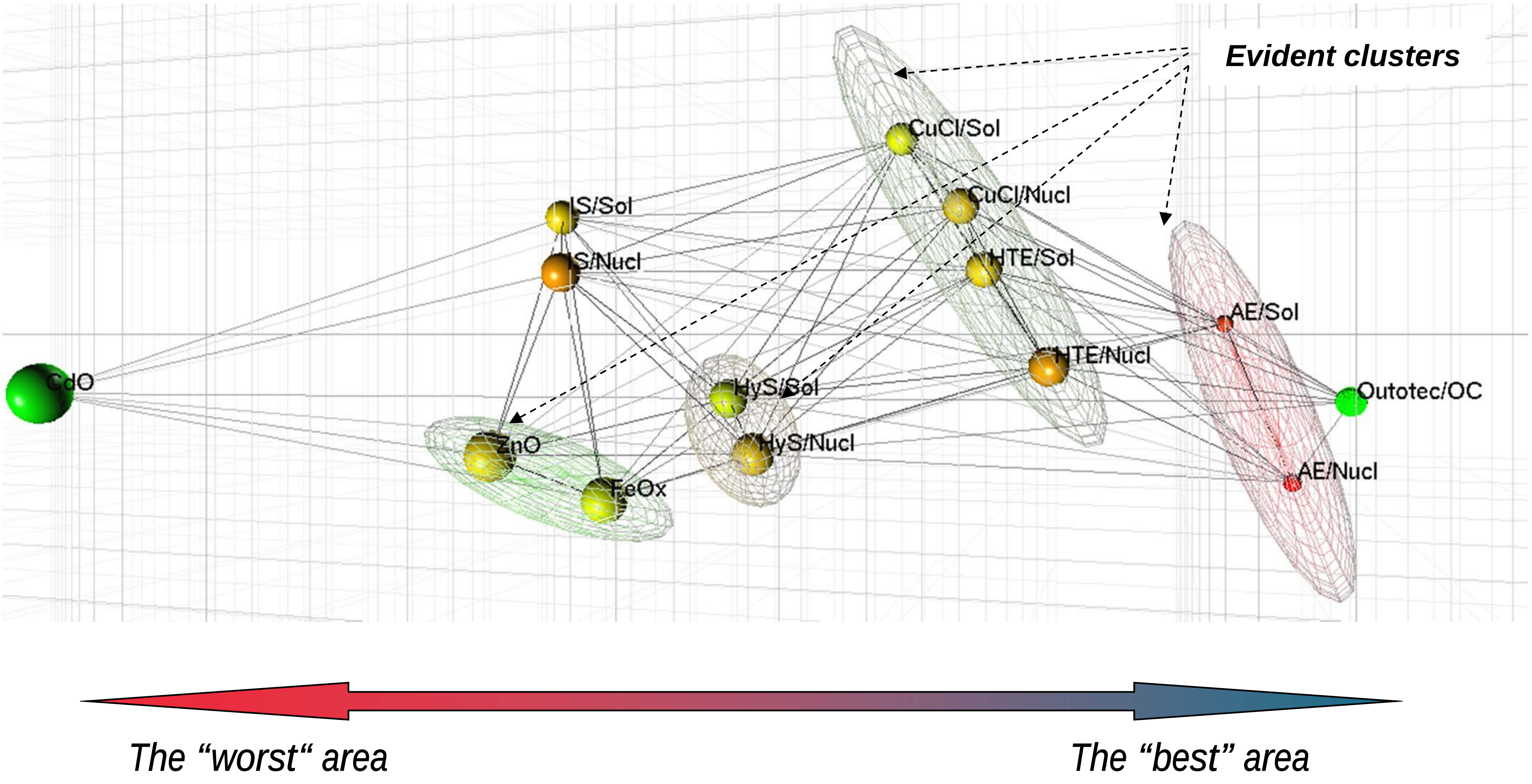
Data must be pre-processed to examine possible errors!

Comparison of thermochemical cycles



Normalized parameters for major H_2 production cycles: AE – alkaline electrolysis, HTE – high-temperature electrolysis, IS – iodine-sulphur, HyS – hybrid sulphur, FeOx – iron oxides cycle; *Sol – solar heat input, Nucl – nuclear heat, Geo – geothermal input*.

Cycles comparison: 3D Euclidian clustering

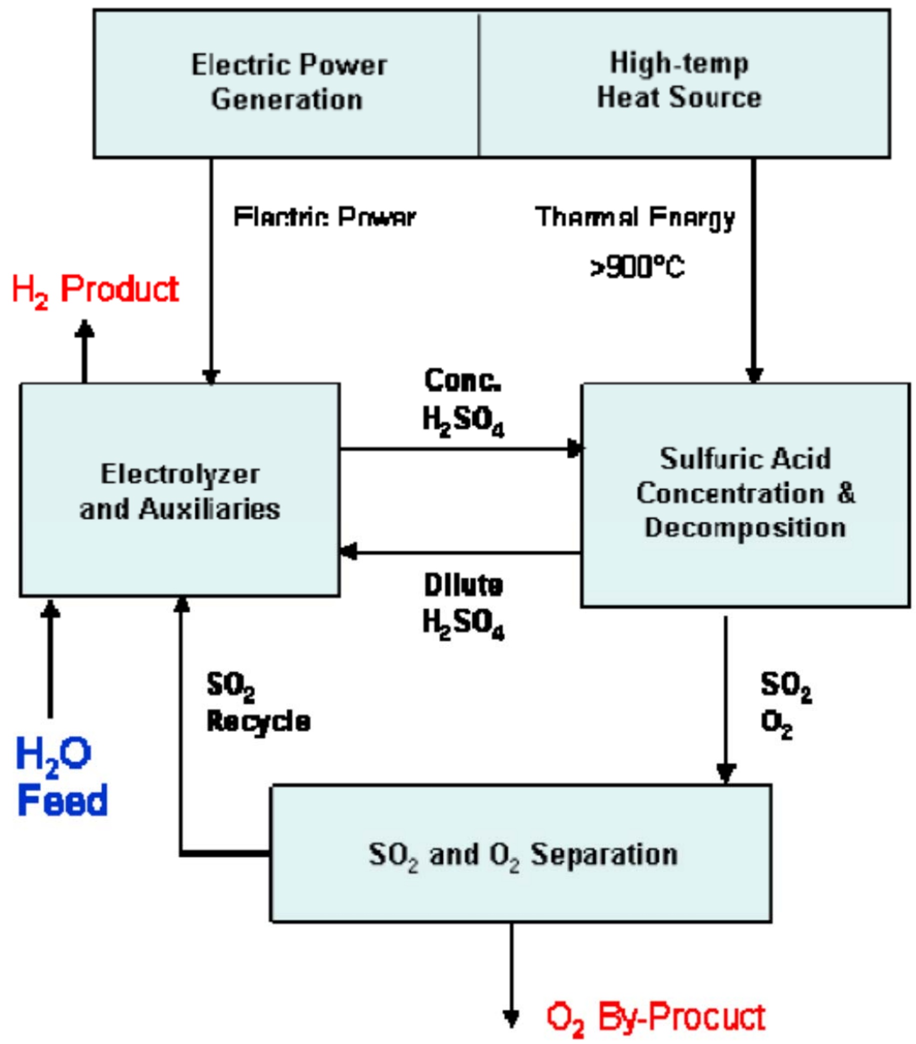


Hybrid sulfur cycle process

- Original idea by Westinghouse
- The key issue:
  - water electrolysis E° = **1.23 V**
  - SO_2 electrolysis E° = **<u>0.17 V</u>** only = **4-5 times less energy than for water!**
- Direct making H_2SO_4 and H_2 at low temperature:

$$\mathbf{SO_2 + 2\,H_2O \rightarrow H_2SO_4 + H_2}$$

- Acid being concentrated and split into SO_2 and O_2 at high-T part *(usually by heat from NPP)*



Why integrated cycles?

BENEFITS:

- more options to efficiently recycle material streams
- efficient share of equipment
- efficient generation and use of utilities
- increased heat integration
- efficient share of treatment facilities, e.g. treatment of waste waters
- reduced bulk storage and, hence, less emissions from storage
- reduced loading/unloading of raw materials and, hence, less emissions
- more options for recycling condensates, process waters, etc.

However:

- integration might decrease the operational flexibility (shutdown for maintenance might cause shutdown of dependent processes)
- Co-products demand and supply might mismatch

SOL2HY2 Project

Topic: SP1-JTI-FCH.2012.2.5

Thermo-electrical-chemical processes with solar heat sources

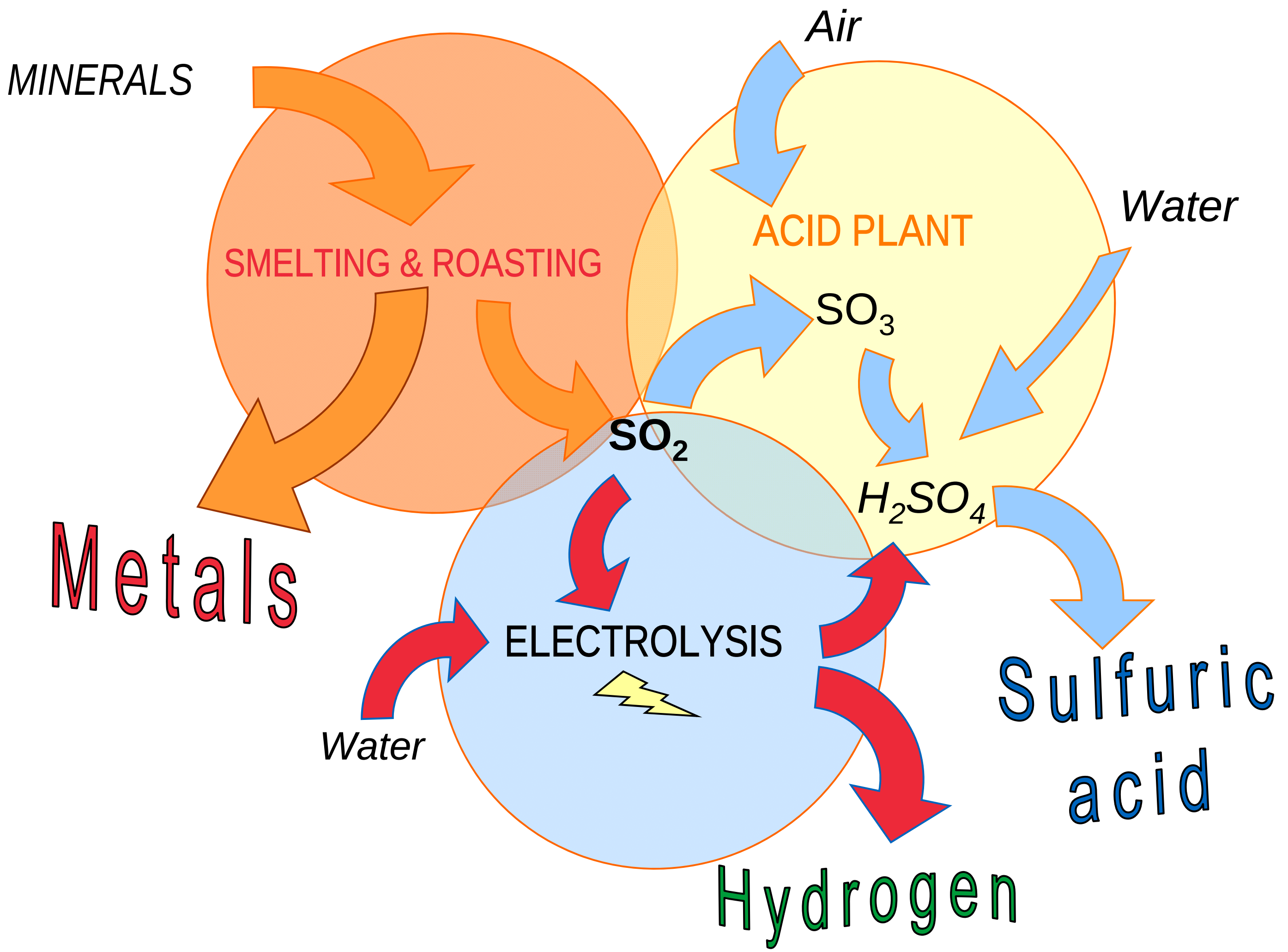
- Basic and applied research on materials and key components for the most efficient thermo-electrical-chemical water splitting cycles
- To improve the technical & economic feasibility of these processes for CO_2-free hydrogen production with focus on the scale up of the technology.
- The solar interface, solar reactors, materials performance and process strategies have been identified as aspects crucial for a reliable and economic operation of a respective plant.

New Energy World JU

fuel cells & hydrogen for sustainability

Fuel Cells and Hydrogen Joint Undertaking (FCH JU)

Key process: Outotec® Open Cycle



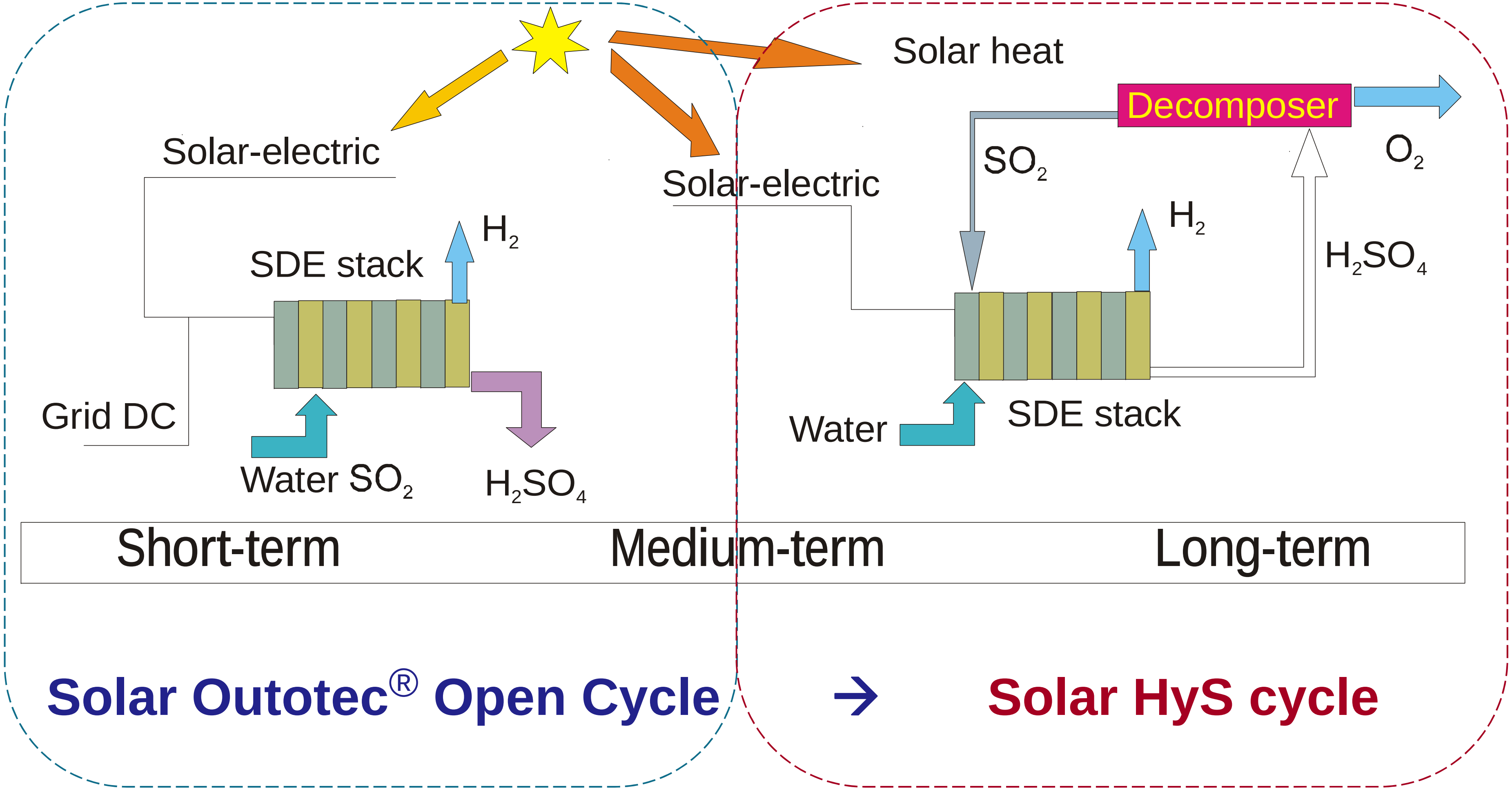
Patented: FI, WO, EA, ZA, US, JP, CN, CA, SA, JR

"The world is not enough" ©

→ Worldwide 22 major Cu smelters: the largest gas output, >25% SO_2 indicates **hydrogen as a by-product** – annually **~223000 t H_2**

- If count ALL the plants – annual potential **30-100 billion Nm^3 H_2**, which is ~10-15% of worldwide industrial H_2 production: Zn, Pb, FeS rosters, H_2SO_4 plants **(250 Mt/y = 5 Mt H_2)**
- **Costs forecast: €0.6-1.0/kg H_2** (recently ~€3-5/kg) at recent material and energy prices (without capital costs and acid sales revenues)
- Almost all stages are tested and industrially verified, costs reduction, optimization and simplification are needed

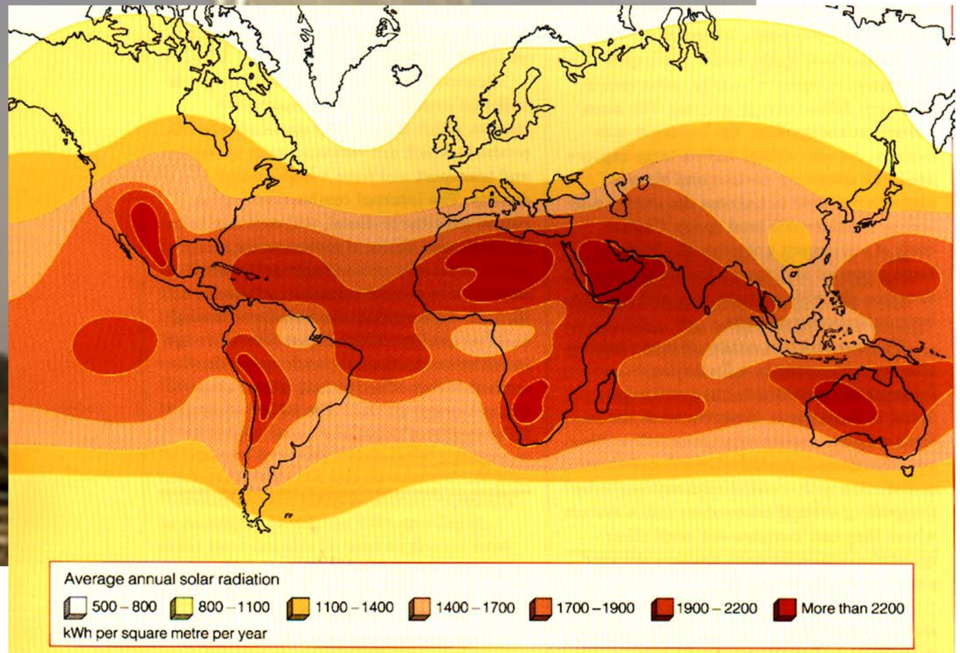
SOL2HY2 project idea:



Solar Outotec® Open Cycle → Solar HyS cycle

Solar tower Jülich

- Receiver 22.7m² (Intratec, Saint-Gobain)
- Tower 60m (Züblin)
- 2150 Heliostats á 8.2 m² (SHP/AUSRA)
- therm. Storage 1h
- Turbine 1.5 MWe (KKK-Siemens)
- Full capacity hours: ca. 1000 h (Storage)
- Electricity Production Energie 1350 MWh/a



Challenges: how CAE can help

- Holistic meta-analysis of technical, chemical, economic and environmental data → combined **H_2 production cycles optimization**
- Solar interface (solar energy, thermal storage, balance of plant) → **improvement** on different levels
- Chemical process engineering → **smart reactor design and operation**
- Key phenomena analysis (species transport, thermodynamics, kinetics) → creation of **engineering meta-models** for plants “green design”

Problems multi-disciplinarity must be properly considered to solve them efficiently!